

Butanoic acid, 3-chloro-

Other names:	Butyric acid, 3-chloro- «beta»-Chlorobutyric acid 3-Chlorobutanoic acid 3-Chlorobutyric acid beta-Chlorobutyric acid
Inchi:	InChI=1S/C4H7ClO2/c1-3(5)2-4(6)7/h3H,2H2,1H3,(H,6,7)
InchiKey:	XEEMVPPCXNTVNP-UHFFFAOYSA-N
Formula:	C4H7ClO2
SMILES:	CC(Cl)CC(=O)O
Mol. weight [g/mol]:	122.55
CAS:	1951-12-8

Physical Properties

Property code	Value	Unit	Source
chl	-2041.80 ± 8.40	kJ/mol	NIST Webbook
chl	-2037.00	kJ/mol	NIST Webbook
gf	-297.31	kJ/mol	Joback Method
hf	-411.72	kJ/mol	Joback Method
hfus	12.48	kJ/mol	Joback Method
hvap	51.92	kJ/mol	Joback Method
log10ws	-0.86		Crippen Method
logp	1.088		Crippen Method
mvol	86.900	ml/mol	McGowan Method
pc	4590.15	kPa	Joback Method
tb	473.96	K	Joback Method
tc	657.92	K	Joback Method
tf	260.51	K	Joback Method
vc	0.328	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	167.29	J/mol×K	473.96	Joback Method
cpg	173.76	J/mol×K	504.62	Joback Method

cpg	179.93	J/mol×K	535.28	Joback Method
cpg	185.81	J/mol×K	565.94	Joback Method
cpg	191.41	J/mol×K	596.60	Joback Method
cpg	196.72	J/mol×K	627.26	Joback Method
cpg	201.77	J/mol×K	657.92	Joback Method
dvisc	0.0347585	Paxs	260.51	Joback Method
dvisc	0.0092852	Paxs	296.08	Joback Method
dvisc	0.0032924	Paxs	331.66	Joback Method
dvisc	0.0014271	Paxs	367.24	Joback Method
dvisc	0.0007170	Paxs	402.81	Joback Method
dvisc	0.0004028	Paxs	438.38	Joback Method
dvisc	0.0002468	Paxs	473.96	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1951128&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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